PORTLAND HARBOR RI/FS

# APPENDIX I

# SURFACE WEIGHTED AVERAGE CONCENTRATION UNCERTAINTY ANALYSIS (PCBS, TOTAL PAHS, DDX)

# FEASIBILITY STUDY

June 2016

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# I1. INTRODUCTION

An evaluation of the uncertainties in predicted post-construction surface sediment COC concentrations was conducted, consistent with the recommendation provided the joint National Remedy Review Board/Contaminated Sediments Technical Advisory Group Comments on the proposed remedy (EPA 2015).

Because predictions of post-construction SWACs are based on a sample from the population of contaminated sediments, statistical uncertainties are unavoidable. In addition, because most remedial investigation data are based on a mixture of sampling designs, some of which are spatially biased accurate estimates of spatial averages must generally be based on weighted averages which are intended to counter the effects of spatially biased sampling designs. In geostatistics this is referred to as de-clustering the data (Isaaks and Srivastava, 2005).

The Portland Harbor FS, data were declustered by first interpolating the concentrations to a 10-foot by 10-foot regularly spaced grid, followed by averaging the values on these grid nodes. This approach based on natural neighbor interpolation has been found to preform reasonably well for reducing bias in SWAC estimates when they are based on a combination of biased and unbiased sampling designs (Kern et al. 2009). The natural neighbor interpolation was also used as a basis to forecast performance of a range of remedial alternatives based on actions taken in areas with the highest interpolated concentrations—referred to as hill-topping. This report documents an evaluation of the uncertainty in these predictions of remedial effectiveness using nonparametric geostatistical procedure known as conditional simulation using the P-field method (Srivastava, 2005).

# I2. METHODS

## I2.1 DECLUSTERING METHOD SENSITIVITY

Prior to conducting the conditional simulation analysis, four declustering techniques were tested to gain an understanding of the sensitivity of SWAC estimates to declustering methods. Methods that were tested included; 1) Thiessen polygons, 2) polygonal declustering, 3) stratified sampling based methods and 4) natural neighbor interpolation.

## I2.2 FUTURE CONDITION

Uncertainty in predicted future condition was evaluated using two approaches; 1) considering basic mathematical constraints relating percentage area remediated, percentage reduction in SWAC and the ratio of remediated to unremediated areas, and 2) using a spatial Monte-Carlo approach to directly estimate confidence limits on post remedial SWAC under a range of remedial action limits (RALs). The first approach is a diagnostic providing a relative understanding of the demands that may be placed on the resolution of the delineation of deposits relative to experiences at other Superfund Mega Sites. The second approach provides a more direct evaluation of the expected remedial performance, under the combination of existing circumstances, including deposit complexity and level of sampling resolution.

### I2.2.1 Mathematical Constraints on Remedial Alternatives

Future condition under selected alternative scenarios was evaluated by considering basic mathematical constraints on the relationships between proportion reduction in post remedial SWAC, the percentage of area remediated, and the ratio of concentrations in remediated to unremediated areas. The constraints are based on equations in **Figure I-1** and provide remedial managers with a relative understanding of the potential level of resolution necessary to achieve remedial targets. In particular, when the remedial footprint is small and the targeted reduction in concentration is large, the ratio of average concentration in remediated areas must be much greater than that in un-remediated areas. This will be feasible, only when high concentration deposits are well-consolidated and easily delineated, or with high density sampling providing highly resolved delineation of otherwise unconsolidated complex depositional patterns.

### I2.2.2 Conditional Simulation

Conditional simulation is a computer intensive resampling method analogous to bootstrap resampling, with the added constraint that rather than randomly selecting individual sample values, whole concentration maps are randomly selected and analyzed (**Figure I-2**). These maps can be thought of as a deck of cards, each of which interpolates the sample data and is also consistent with the spatial variation observed in the sample. The analysis proceeds by randomly selecting one of many equally likely maps to which proposed remedial strategies are applied. The results for each randomly selected map are summarized, providing a means to propagate spatial variation and uncertainty through complex calculations, linking uncertainty in maps with uncertainty in SWAC predictions.

The technique takes into account the spatial uncertainty in mapped surfaces, and is spatially scalable and also accounts for uncertainty in the delineation boundaries. Uncertainty calculations help to quantify the effects of the situation where some contaminant concentrations within the RAL footprint are less than the RAL, as well as the when some concentrations outside the footprint may be greater than the RAL. These types of errors are assumed negligible when forecasts are based purely on a single smooth surface which can lead to inaccurate evaluations, usually biased toward overstatement of remedial benefit. This analysis provides an assessment of how these uncertainties accumulate in the post remedial SWAC predictions.

**Detailed P-Field Simulation Procedure (Optional Reading)**
The P-field simulation method involves three primary steps; 1) defining conditional cumulative distributions for COCs at each 10 by 10 foot grid cell, 2) simulating a spatially correlated normally distributed random variable for each grid cell, and 3) transforming the normally distributed variable to the original COC scale by identifying the percentile of the COC distribution with corresponding percentile of the simulated normal random variable at each grid cell. The cumulative distributions represent narrower ranges near sample values and wider ranges far from sample values, causing the simulated surfaces to match measured values at the sampled locations, whereas they may vary relatively widely in areas that are distant from sampled locations.

The conditional cumulative distribution functions were estimated using a nonparametric approach based on natural neighbor interpolation approximating the indicator kriging method that is typically used to estimate cumulative distribution functions. Estimating conditional distributions requires interpolation of a range of binary (0 or 1) indicators defined based on COC concentrations being above or below a range of threshold values of interest. In this analysis threshold values were chosen to represent percentiles of the COC distributions, (1, 2.5, 5, 10, 20, 30, 40, 50, 60, 70, 80, 90, 95, 97.5 and 99). For each percentile, the sample data were coded as 1 for values below threshold and 0 for values above threshold, and these binary values were interpolated using natural neighbor interpolation. This process was repeated for each of the 15 threshold values, resulting in 15 interpolated surfaces representing the probability that COC concentrations were less than the threshold value. This series of 15 probability values unique to each grid cell is an estimate of the conditional cumulative distribution at that location. Traditionally this interpolation is conducted using indicator kriging. However, using natural neighbor interpolation has two distinct advantages, there is no need to model 15 sets of directional indicator variograms necessary for kriging,, and the natural neighbor method does not require any assumptions of stationarity as is assumed for kriging. Effectively by using the natural neighbor method to interpolate the indicator data, the resulting simulation is both non-parametric as well as accommodating spatially nonstationary COC distributions.

# I3. RESULTS

## I3.1 DECLUSTERING METHOD SENSITIVITY

Estimated SWACs for PCBs based on four declustering methods ranged from 79 µg/kg for the method stratified on RAL areas, to 205 µg/kg based on unweighted averages within geographic strata. The stratified method based on Thiessen Polygon weighting was 135 µg/kg, and the method stratified based on RAL areas and using Thiessen Polygon weighting was similar to the natural neighbor method deployed in the FS. As shown, the effects of biased sampling are substantial, with higher unweighted estimates reflecting tendency to focus sampling on high concentration areas. This indicates that some form of declustering is appropriate to improve the accuracy of estimates which would otherwise be based on an unweighted average.

## I3.2 MATHEMATICAL CONSTRAINTS

The planned percentage SWAC reduction was plotted against percentage area remediated for PCBs to evaluate the susceptibility of remedial alternatives identified in the FS to delineation errors, and to compare with other remedial alternatives implemented at a number other Superfund Sites (**Figure I-3**). Alternatives E and G each require that the ratio of average SWAC within remediated to unremediated areas should be approximately a 10 to 1 ratio—both alternatives falling roughly along the red 10 to 1 curve. Other sites that have deployed similar ratios, include the Fox River OU4-5 and River Section 2 of the Hudson River. The results at the Fox River Site are not yet complete; however, the deposits there were relatively broadly distributed and only mildly consolidated and ultimately substantial design sampling has been required to achieve this goal. Conversely, deposits in River Section 2 of the Hudson River Site are better consolidated, but not as well consolidated as is apparent in Portland Harbor, and the desired outcome was not fully achieved there. Based on qualitative observation of the distribution of surface COCs at Portland Harbor, it is anticipated that this 10 to 1 ratio is likely to be achievable with substantially less resolution than was required at the Fox River Site, and potentially similar sampling densities to those deployed at the Hudson River in River Section 2. The conditional simulation will help to test this observation more rigorously.

## I3.3 CONDITIONAL SIMULATION

Conditional simulation was used to estimate uncertainty in the SWAC vs RAL relationship. The RAL was varied for each COC representing remedial action limits associated with alternatives B through G described in the FS (**Table I-2**). The lateral footprint for each RAL was defined by all grid cells with natural neighbor interpolated concentrations exceeding each specified RAL.

To simulate remediation, remediated cells were replaced with expected background concentrations and SWAC was calculated by averaging all cells (remediated and un-remediated) in the map

Four equally likely simulated maps of PCB concentration are shown in **Figure I-4** to illustrate the level of variation that may occur between maps, but that is nonetheless consistent with the sample data. The RAL boundaries for Alternative E, established from the smooth natural neighbor interpolation, are overlaid so that it can be seen that for some maps, areas outside the remedial footprint exceed the 200 µg/kg threshold and that in some areas for some maps concentrations inside the remedial footprint may be less than the RAL. Generally areas within the RAL footprints tend to be similar among all four maps; however, some areas outside the footprint tend to vary substantially, as indicated by the callouts in the left two panels. This reflects the greater sampling density within the deposits relative to somewhat lower sampling density within the navigation channel, where concentrations are lower and inaccuracies in delineation have less effect on remedial effectiveness.

Conditionally simulated SWACs for PCB concentrations varied from approximately 67 to 95 with an average of 79 prior to remediation, which was equal to the SWAC estimated from the average of the natural neighbor surface (**Figure I-5**). These values were equal because the simulation algorithm is intentionally constrained so that the synthetic mean is required to match the declustered SWAC based directly on sample data.

This range is also portrayed on **Figure I-6**, depicted as a gray band surrounding the pre-remedial SWAC estimate. The simulated SWAC distribution, depicted as red squares with error bars shows that as expected SWAC declines with lower RALs. Additionally, the uncertainty bounds on SWAC is narrower for lower RAL values reflecting that a larger remedial footprint both reduces the SWAC but also its uncertainty. Action limits of 750 µg/kg and 1,000 µg/kg had higher uncertainties, with remedial benefit potentially within the margin of error, as indicated by the overlapping uncertainty bounds with the pre-remedial SWAC. Post remedial SWAC for total PCB is clearly outside the margin of error of pre-remedial SWAC indicating clear expectations that the predicted remedial benefit is likely to be achieved in practice.

Pre and post remedial total PAH and DDx concentrations in relation to action limits are plotted on **Figure I-7** and **Figure I-8** respectively. These distributions are characterized by similar qualitative patterns to those observed for PCBs. Relative error is generally greater for these COCs than for PCBs which had greater skewedness in the PAH and DDx distributions, relative to the PCB distribution. Notably, the effects of this uncertainty are minimized in the post remedial forecasts where these areas are remediated under any RAL considered, and therefore their influence is eliminated from the analysis. These RAL and corresponding SWAC values are also summarized in **Table I-3**.

# I4. DISCUSSION

Surface weighted average concentration is an estimate exposure to receptors which may range over large areas. If sampling were purely unbiased, standard estimation methods for the mean and its confidence interval would be appropriate and less computationally complex. Because the sample data are right skewed, nonparametric, as opposed to normal theory, methods are preferred irrespective of the sampling design. If the sampling design had been unbiased, one could select one of the bootstrap based methods provided in ProUCL for estimating the mean and it is UCL. However, with biased sampling prevalent at Portland Harbor it is necessary to spatially weight the data in order reduce bias in the estimated mean and to properly characterize uncertainty bounds. Conditional simulation, is a variant of bootstrapping for designed to accommodate biased sampling designs and data that are spatially correlated.

The gray band on **Figures I-6** through **I-8** represents the 95 percent confidence interval for the pre-remedial SWAC, and the error bars represent 95 percent prediction intervals for the post remedial SWAC corresponding to each RAL. When these intervals do not overlap, one can be more than 95 percent confident that the pre and post remedial means would differ ($p<0.05$). When one error bar overlaps the mean there is no difference at the 5 percent level of confidence ($p>0.05$) and when error bars overlap slightly, one can conclude that there are differences but that the confidence level may be somewhat less than 95 percent. Generally, any RAL which results in an estimated SWAC with error bars that do not overlap the confidence limits of the pre-remedial SWAC can be expected to reliably result in reduced post-remedial concentrations within the range of values bounded by the confidence limits.

It should also be noted that as the RAL declines, the error bars also decline. This is because the variance the change in SWAC is proportional to the square of the proportion of area remediated.

$$var(\Delta SWAC) = (Proportion\ Remediated)^2 \times var(\Delta Concentration)$$

Simply, as the size of the remedial footprint grows, the chance of making delineation mistakes declines with the area remediated. If the entire site is remediated, there is no uncertainty.

# I5. REFERENCES

EPA, 2015. National Remedy Review Board and Contaminated Sediments Technical Advisory Group Recommendations for the Portland Harbor Superfund Site. Office of Solid Waste and Emergency Response. December 31, 2015

Isaaks, E. and R.M. Srivastava. 2005. *Introduction to Geostatistics*, Oxford University Press. New York.

Kern, J.W. 2009. Geostatistical conditional simulation for incorporating uncertainty into SWAC-based remedial selection. Fifth international conference on remediation of contaminated sediments. Jacksonville, FL.. https://www.researchgate.net/publication/236585034_Geostatistical_Conditional_Simulation_for_Incorporating_Uncertainty_into_SWAC_Based_Remedy_Selection. Last accessed 4/14/2016.

Srivastava, R.M. 2005. Probability field simulation: A retrospective. In: *Geostatistics Banff, 2004., 55-64.* Springer, Netherlands.

# Tables

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**Table I-1**
**Declustering Method Sensitivity for PCBs**
Portland Harbor Superfund Site
Portland, Oregon

| Declustering Method | SWAC Estimates PCBs (µg/kg) |
|---|---|
| Stratified and Unweighted | 205 |
| Stratified on Geographic areas with Thiessen Polygons | 135 |
| Stratified on RAL Areas with Thiessen Polygons | 79 |
| Polygonal Declustering | 105 |
| Average Natural Neighbor Map | 80 |

**Table I-2**
**RALs for Remedial Options B through G for PCBs, Total PAH and DDx**
Portland Harbor Superfund Site
Portland, Oregon

| COC Name | Units | Remedial Option | | | | | |
|---|---|---|---|---|---|---|---|
| | | B | C | D | E | F | G |
| PCBs | µg/kg | 1,000 | 750 | 500 | 200 | 75 | 50 |
| Total PAHs | µg/kg | 170,000 | 130,000 | 69,000 | 35,000 | 13,000 | 5,400 |
| DDx | µg/kg | 650 | 550 | 450 | 300 | 160 | 40 |

**Table I-3**
**Predicted Post Remedial SWAC (µg/kg) for a RALs.**
Portland Harbor Superfund Site
Portland, Oregon

| COC | RAL | 95% Lower Confidence Limit | SWAC | 95% Upper Confidence Limit |
|---|---|---|---|---|
| PCBs | 50 | 22 | 24 | 25 |
| | 75 | 27 | 28 | 30 |
| | 100 | 30 | 32 | 34 |
| | 200 | 37 | 42 | 46 |
| | 500 | 48 | 55 | 64 |
| | 750 | 53 | 61 | 72 |
| | 1,000 | 56 | 65 | 77 |
| Total PAHs | 5,400 | 2,082 | 2,580 | 3,116 |
| | 13,000 | 2,899 | 3,882 | 4,845 |
| | 35,000 | 3,979 | 5,618 | 7,251 |
| | 69,000 | 4,518 | 6,817 | 9,405 |
| | 130,000 | 5,479 | 8,641 | 13,035 |
| | 170,000 | 6,054 | 9,539 | 14,980 |
| DDx | 40 | 13 | 16 | 19 |
| | 160 | 19 | 24 | 33 |
| | 300 | 21 | 28 | 43 |
| | 450 | 23 | 33 | 55 |
| | 550 | 23 | 35 | 64 |
| | 650 | 24 | 38 | 71 |

# Figures

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$A_U$ –Unremediated Area

$C_U$--Unremediated Concentration

$A_R$ –Remedial Area

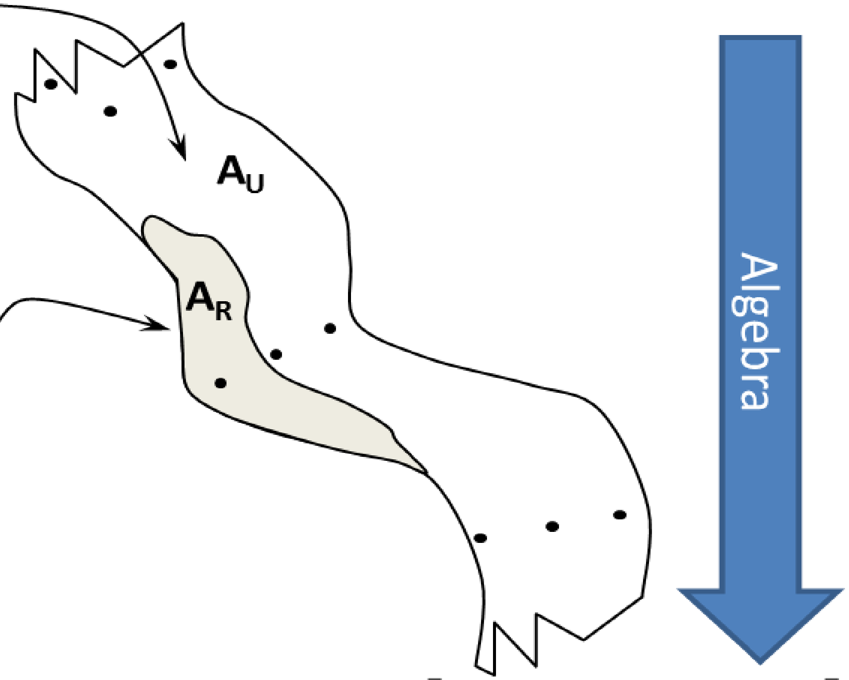
$C_R$-Remedial Footprint Concentration

$C_{Residual}$ -Post-remedial Concentration

$$R_A = A_R/(A_R + A_U)$$

$$R_C = C_R/C_U$$

$$SWAC = \frac{(A_U \times C_U + A_R \times C_R)}{A_U + A_R}$$




$$\frac{\Delta SWAC}{SWAC} = R_A \left[ \frac{1 - \frac{C_{Residual}}{C_R}}{R_A + (1 - R_A)/R_C} \right]$$

**Figure I-1. Mathematical Relationships Governing Remedial Performance**

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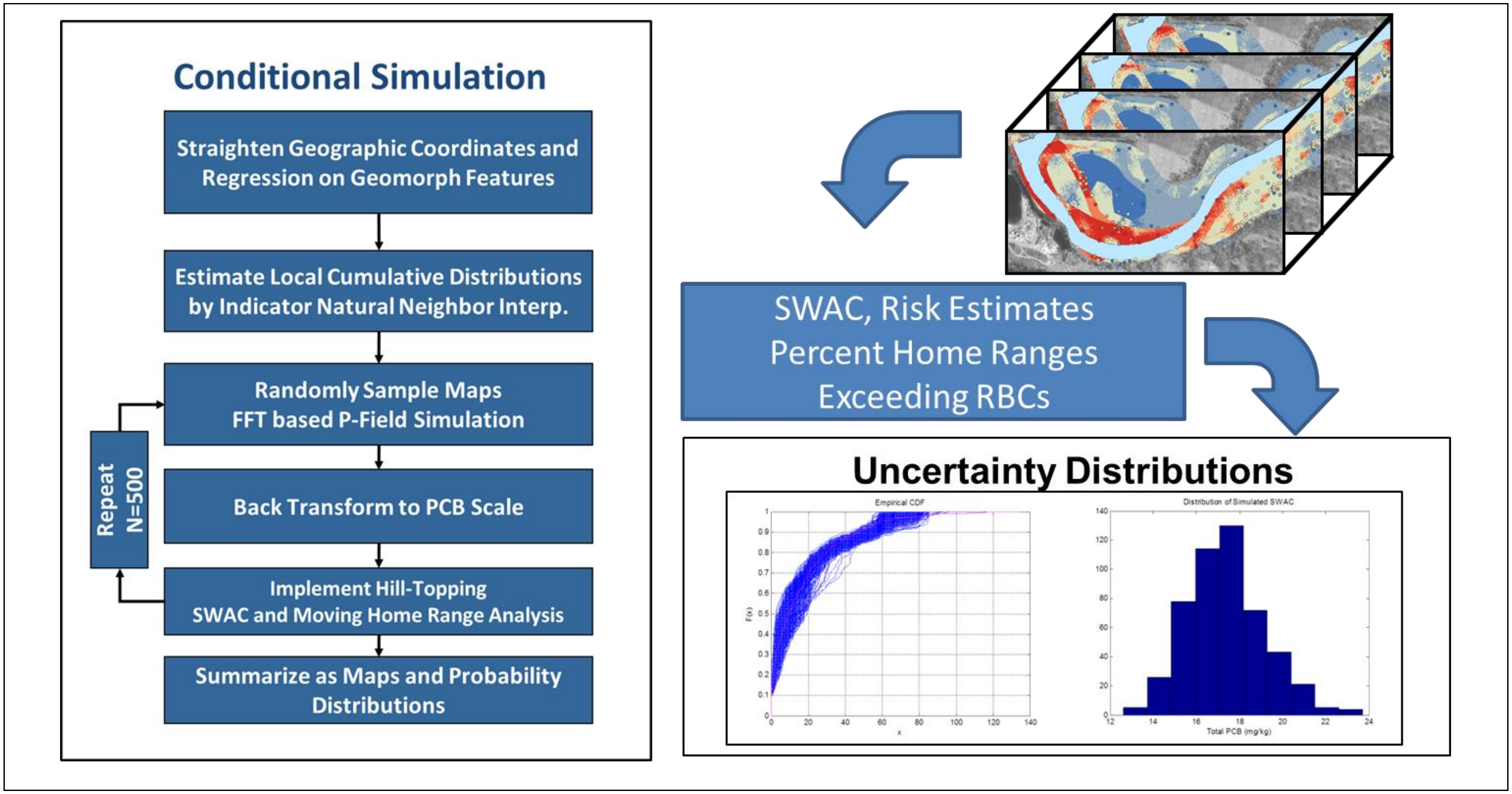


**Figure I-2. Conditional Simulation Procedure**

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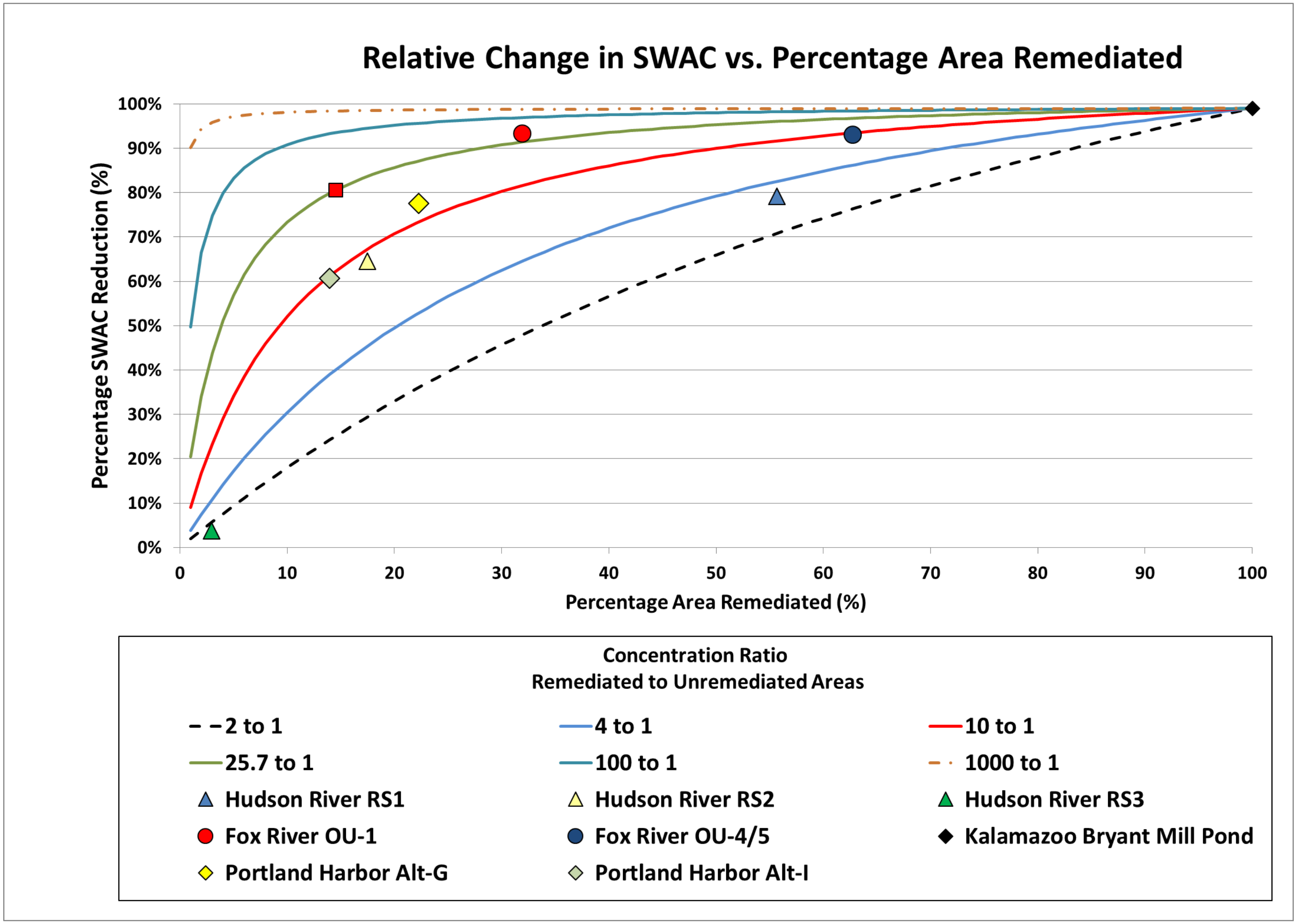


**Figure I-3. Relative Change in SWAC vs Percentage Area Remediated**

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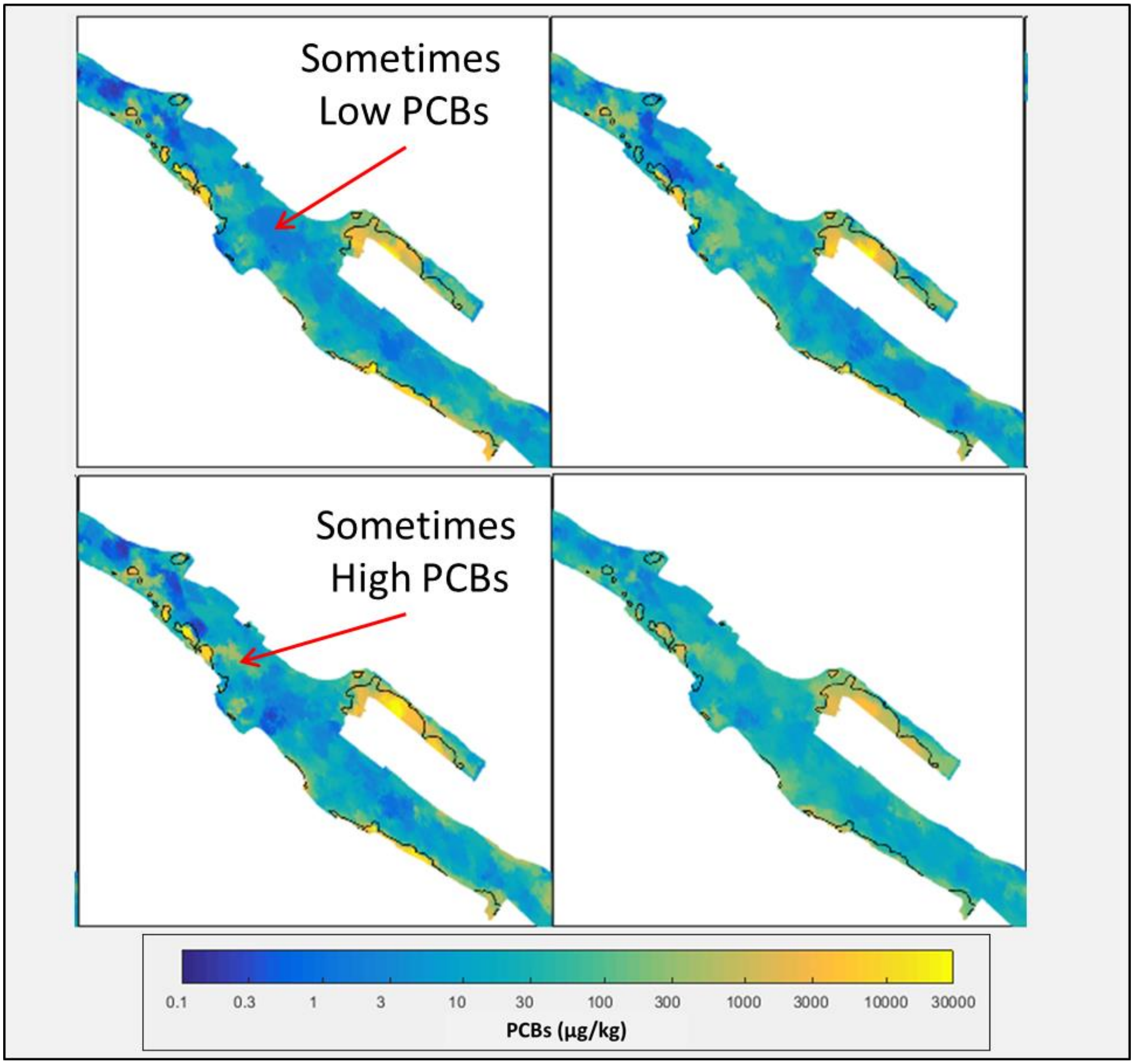


**Figure I-4. Four Equally Likely Simulated Maps of PCBs**

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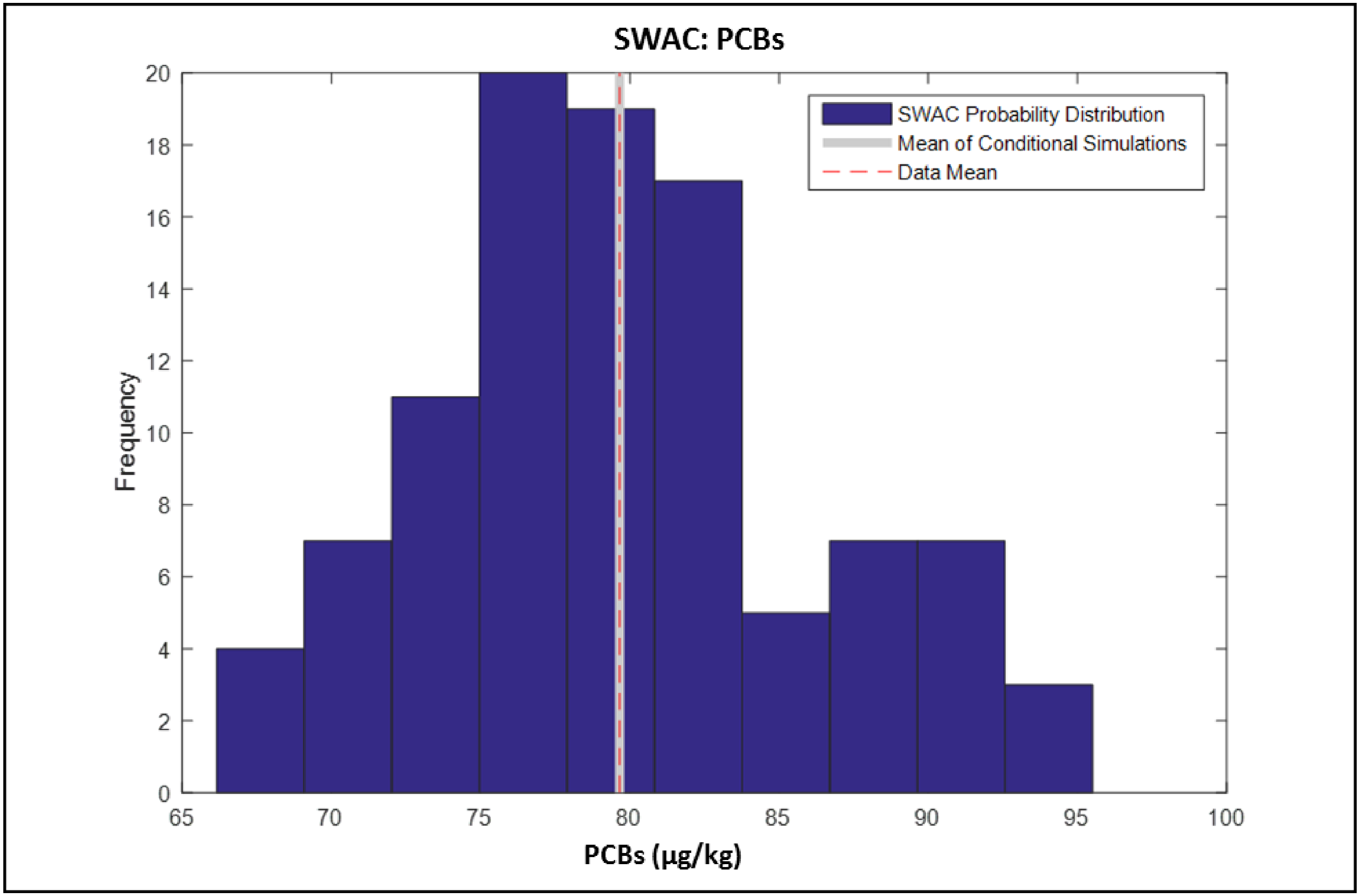


**Figure I-5. Pre-Remedial SWAC - PCBs**

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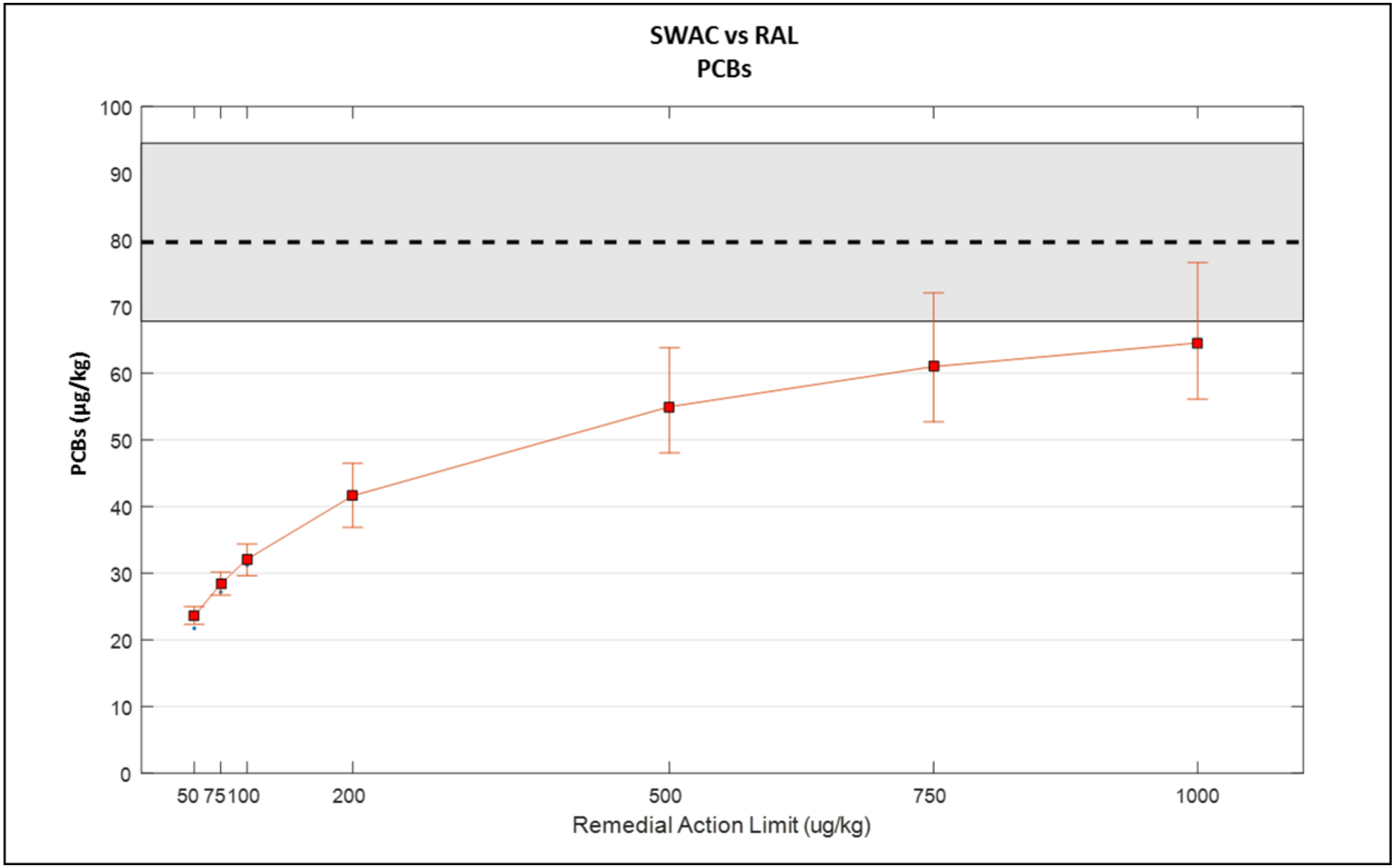


**Figure I-6. Surface Weighted Average Concentration for PCBs vs. RALs**

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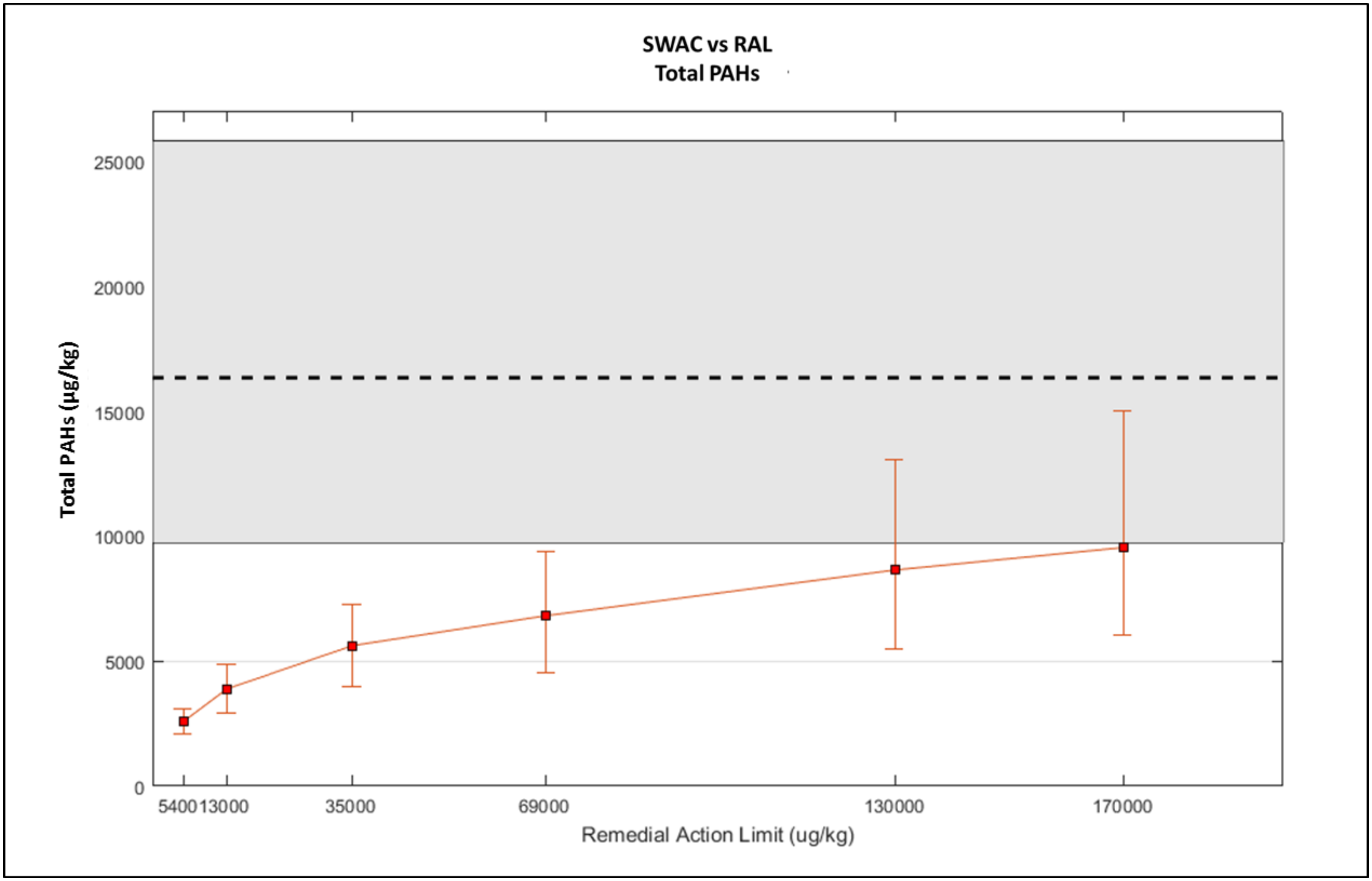


**Figure I-7. Surface weighted average concentration for Total PAHs vs. RALs**

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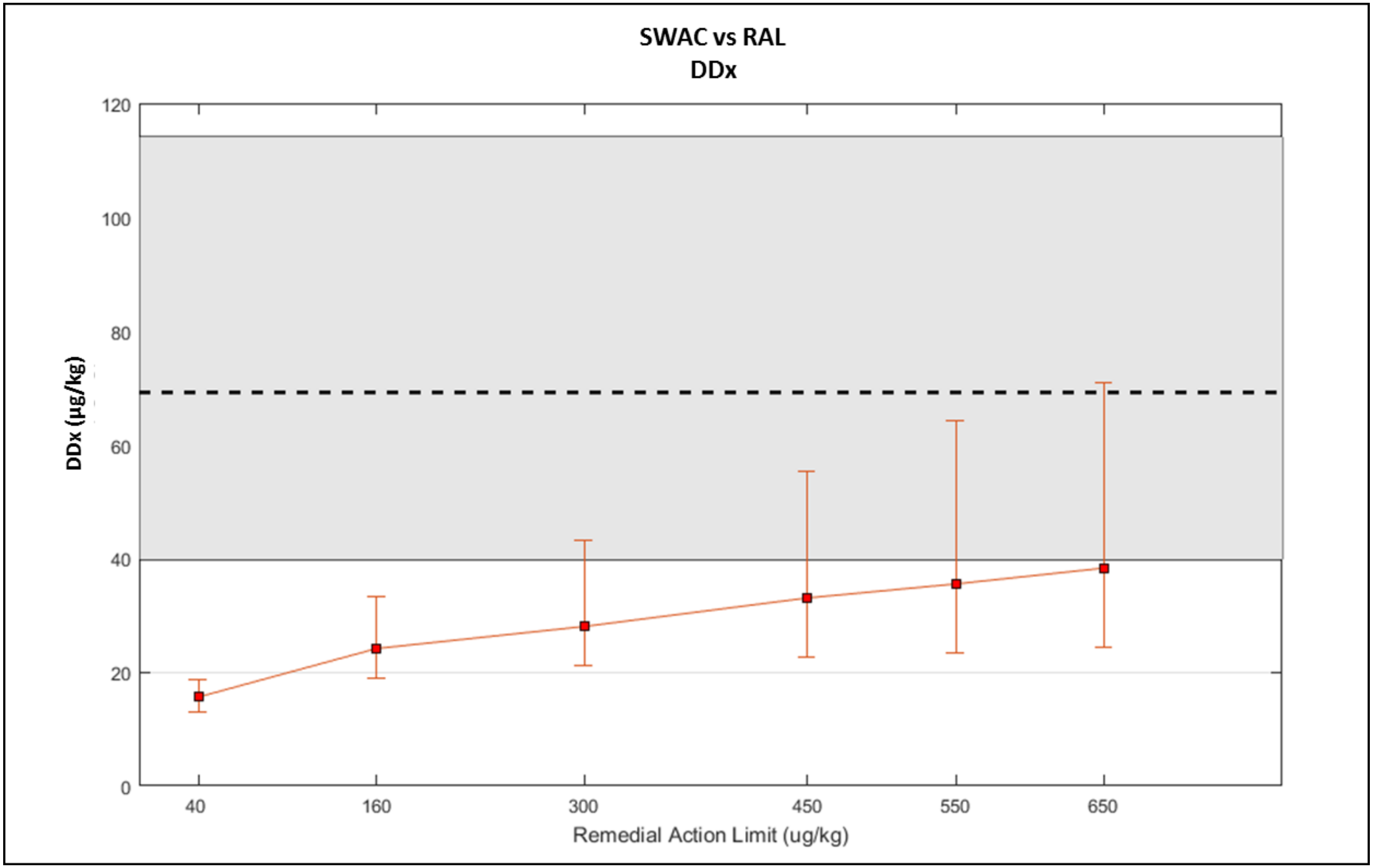


**Figure I-8. Surface Weighted Average Concentration for DDx vs. RALs**

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